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Title: LANL Capabilities for Opioid Screener (DHS proposal preparation with QFS)

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# LANL Capabilities for Opioid Screener

Team: Michael Janicke ( $^{14}\text{N}$  NMR), Michelle Espy (FFC cross-relaxation), Michael Malone ( $^{14}\text{N}$  NQR), Tammie Nelson (DFT computations), Robert Williams (National Isotope Resource, DEA license), Derrick Kaseman (solid-state NMR)

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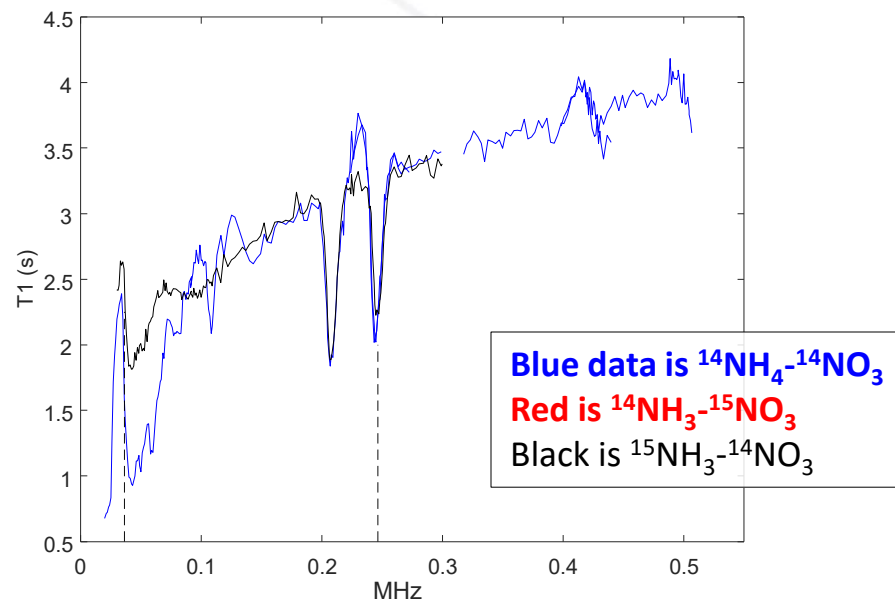
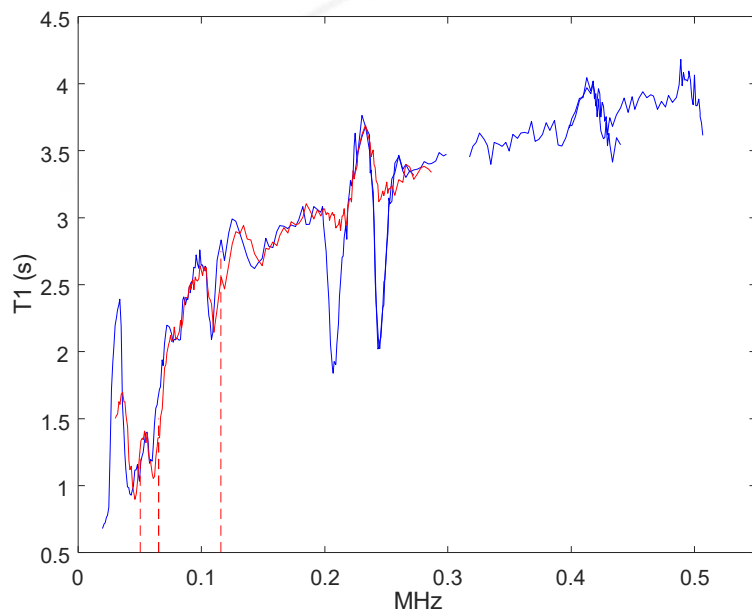
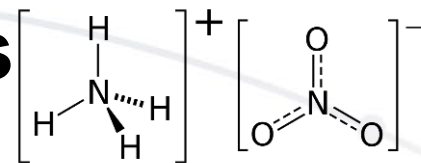
# Capabilities

- Access to controlled substances and safety procedures in place for examining fentanyl and other synthetic derivatives with Laboratory DEA license (Williams)
- Previous experience with  $^{14}\text{N}$  NMR and NQR detection of energetic materials (Malone and Espy)
- Fast Field Cycling (FFC) NMR instrument for determining  $^{14}\text{N}$  NQR frequencies (Espy, Janicke and Malone)
- $^{14}\text{N}$  high field solid-state NMR instrument for corroborating FFC results (Janicke and Kaseman)
- DFT calculations for  $^{14}\text{N}$  NQR and NMR parameter predictions (Nelson)
- Chemistry facilities for isotope enrichment ( $^{15}\text{N}$  replacement for understanding nitrogen spectroscopic signatures), sample synthesis, material preparation, and safe storage (Williams)
- Facilities for field testing  $^{14}\text{N}$  NQR systems (Malone)

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# Previous LANL $^{14}\text{N}$ NQR success

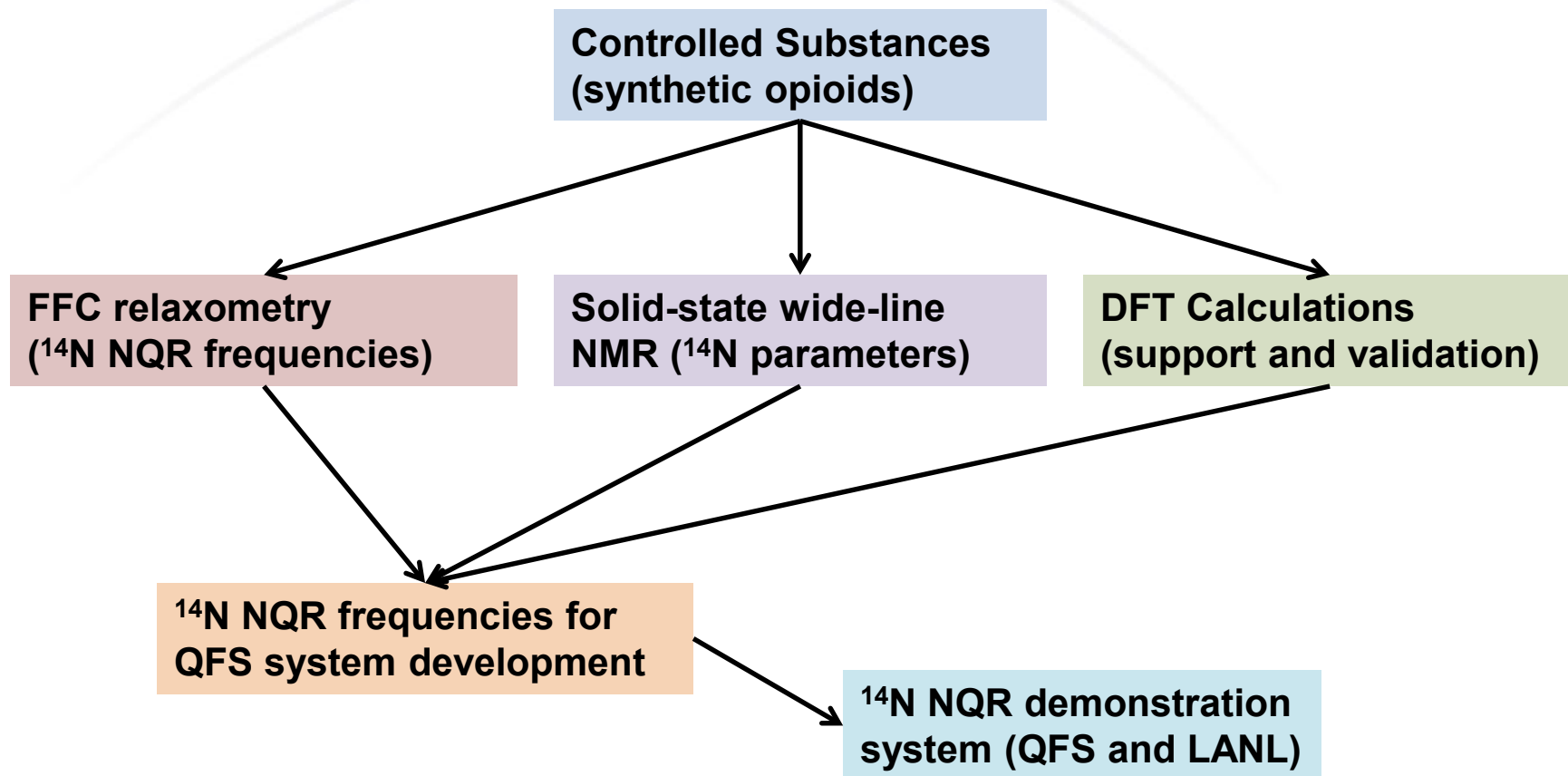


- LANL ammonium nitrate cross relaxation study ( $\text{NH}_4\text{-NO}_3$ ) from FFC relaxometer, plotted are the changes in relaxation properties ( $T_1$ ) with magnetic field (MHz)
- Features in the  $T_1$  curve correspond to observed NQR frequencies and half frequencies
- Isotopic enrichment assists in simplifying overlapping signals from multiple nitrogen sites in compounds, such as fentanyl and carfentanil

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# LANL Roadmap



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